

# Application of thermodynamic modeling in the steel metallurgy

Z. Taszner, J. Rudnizki – GTT Workshop, September 14 – 16, 2011



**ThyssenKrupp Steel Europe**  
Rohstahl / Qualitätswesen und Verfahrenstechnik



**ThyssenKrupp**

# Agenda

- Introduction

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- Thermodynamic application at TKSE

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- FactSage - application examples
  - Solubility limits in TBM-steel

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  - Precipitation reactions

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  - Solidification of peritectic steels

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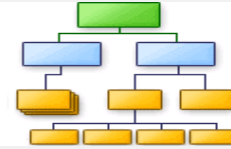
  - Heat balance calculations for BOS

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  - Phase diagrams for slag systems

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**Dr. Müller**  
QuV

**Dr. Petry**  
Process Development

**Dr. Rudnizki**  
Projects  
Metallurgy

**Shepherd**  
Projects  
Metallurgy

**Dr. Taszner**  
Projects  
Metallurgy

### Responsibilities (Process Development)

- Technological support for steel production
- Metallurgical process optimization, thermodynamic modeling
- Development and supply of engineering tools for the process and quality control

**Beirer**  
Quality Control

**Fiedler**  
Quality Control  
external/CSA

**Linneweber**  
Quality Control  
Ox2

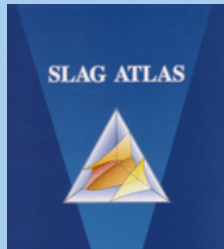
**Dr. Toulouse**  
Quality Control  
Ox1



# Thermodynamic tasks and applications at TKSE

Steel metallurgy

Materials engineering



DICTRA



Thermo-Calc Software

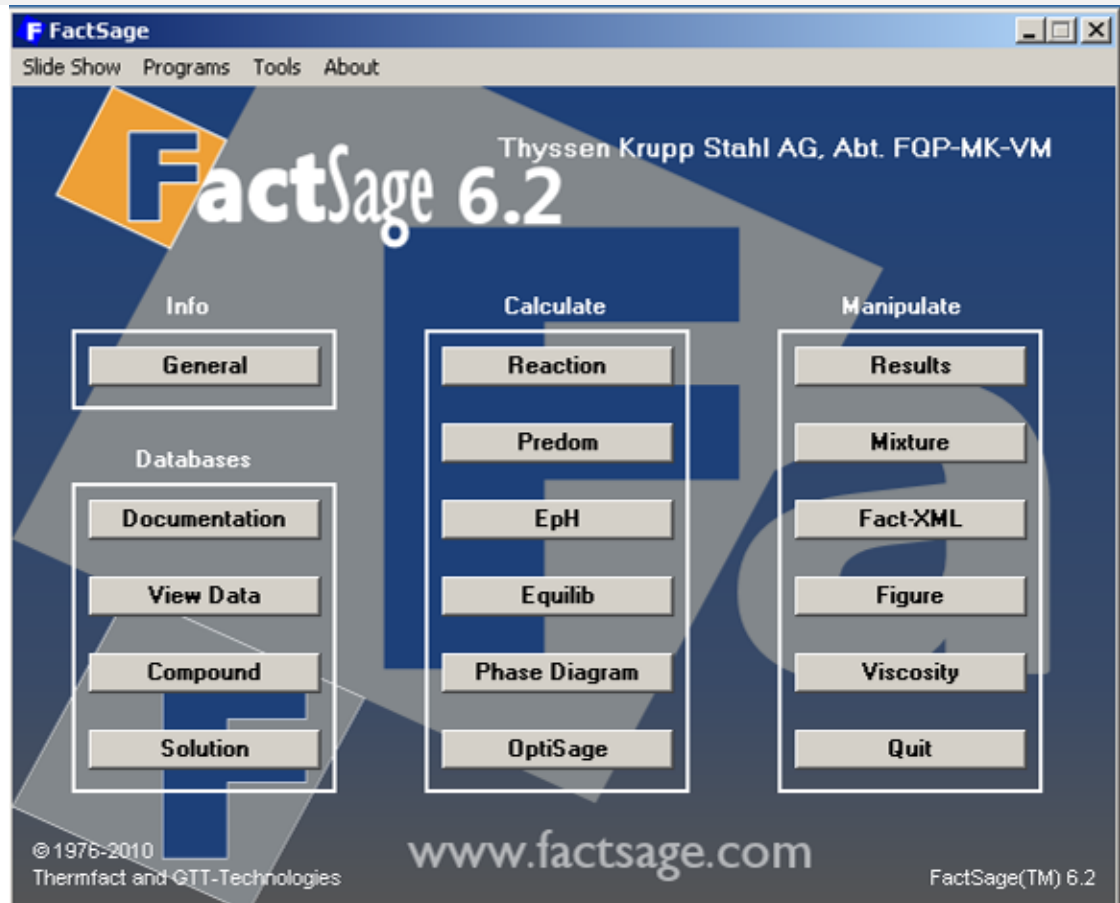
FactSage:

Calculation of thermodynamic functions, phase diagrams, equilibria and reactions in steels and slags, mass and heat balances



# Software: FactSage (Network)

- Thermodynamic databases
  - phase diagrams
  - reactions
  - equilibrium
  - slag viscosity
- Data set optimization
- Visualization



<http://www.gtt-technologies.de/>

<http://www.factsage.com/>



FactSage  
07.10.2011  
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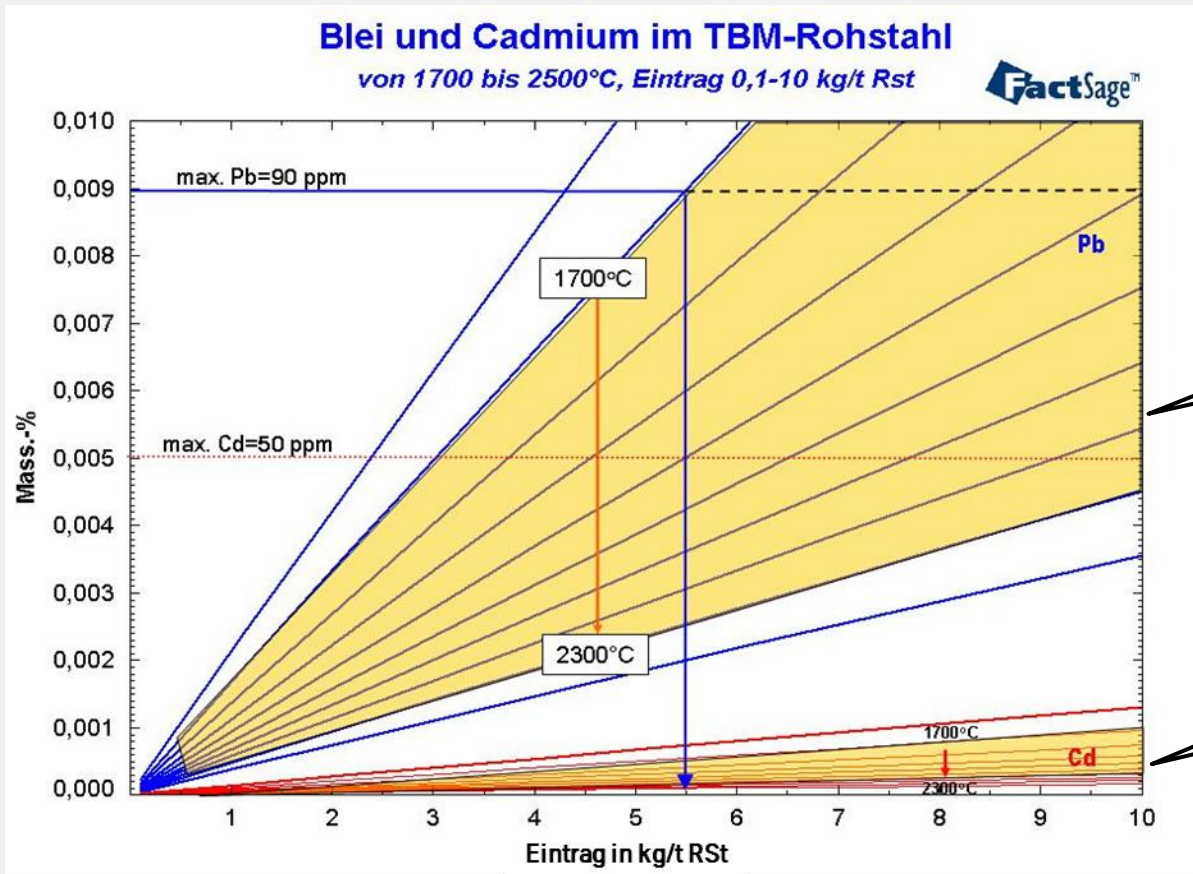
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# Application example: Solubility limits in TBM-steel

- Study for the compliance of the concentration limits according to customer request of 90 ppm Pb and 50 ppm Cd in TBM-steel



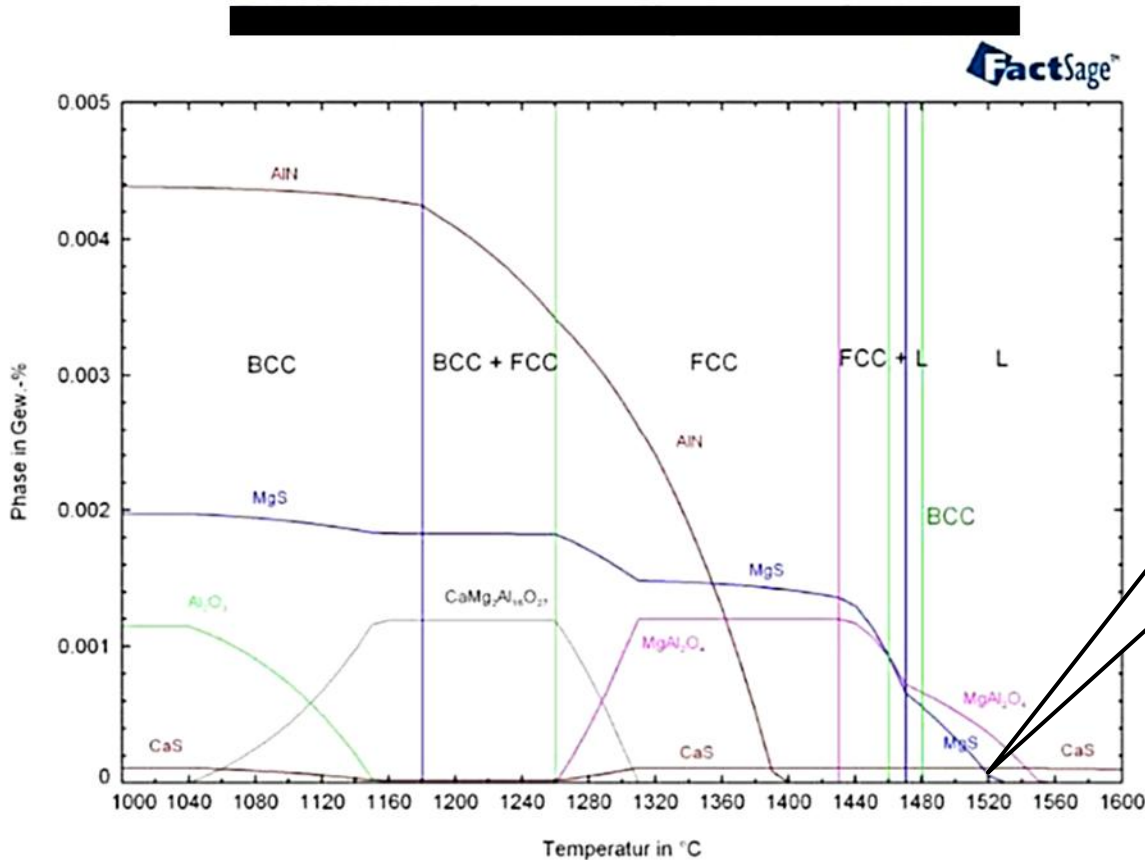
Maximum solubility of 90 ppm Pb at 1700°C can not be achieved by BOF process. An input of ca. 5,5 kg/t heavy metal is not realistic.

50 ppm limit for Cd could not be reached under reasonable metallurgical assumptions.



# Application example: Precipitation reactions

- Contribution to the determination of relationship between change in the magnetical properties of electrical steels and non-metallic inclusions

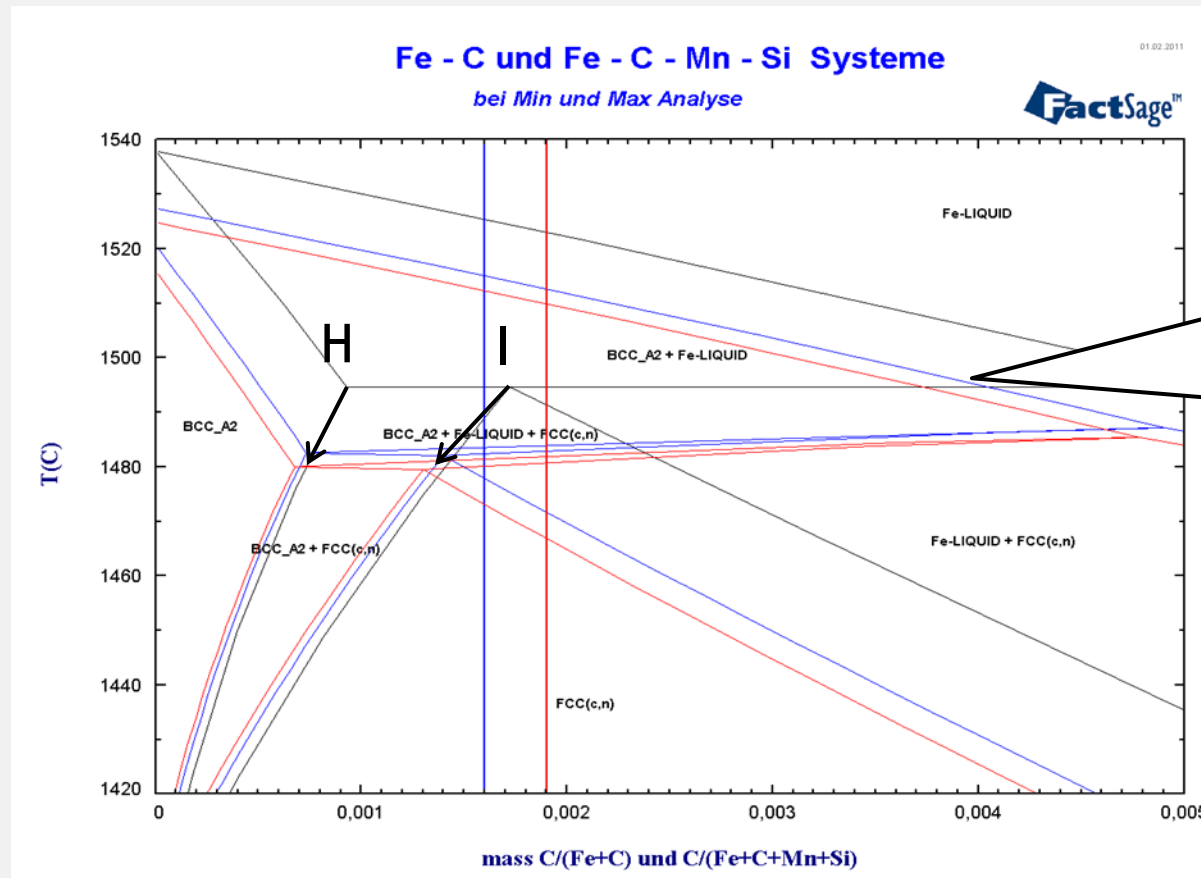


MgS is thermodynamically stable below 1520°C. Critical configurations of MgS can be avoided by reducing the Mg-content.



# Application example: Solidification of peritectic steels

- Determination of specific influences of alloying elements on the C-equivalent using phase diagrams



Prediction of the peritectic behaviour and prevention of the critical concentrations by adjusting the chemical composition



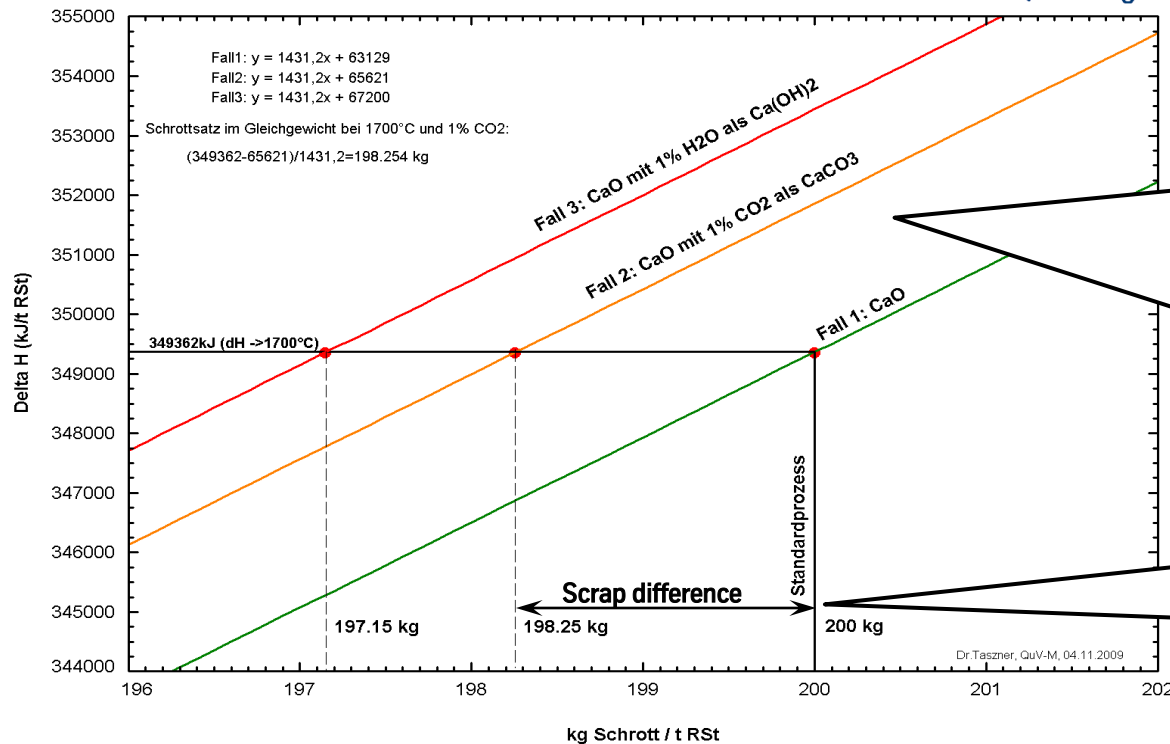


# Application example: Heat balance calculations for BOS

- Detection and quantification of negative influences of „lime-burning“ on the scrap proportion in the oxygen blowing process

## Schrottäquivalenter Energiebedarf des Kalkbrennens im Konverter

1t Stahl mit 40kg CaO bei 1700°C



- case 1:  
scrap/crude steel equilibrium with normal lime
- case 2:  
equilibrium with not fully burned lime (1% CO<sub>2</sub>)
- case 3:  
equilibrium with not fully burned lime (1% H<sub>2</sub>O)

not fully burned lime reduces scrap amount in converter which must be compensated by hot metal





# Thank you for your attention!



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